MLS000736649

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 25.7

Global applicability domain: Inside

Local applicability domain index: 4.72e-01

Confidence level: 5.70e-01

Nearest Neighbors from the Training Set

Image not found

Isoamyl ether
Measured: 170
Predicted: 137

Image not found

N,N-Diethylaniline
Measured: 102
Predicted: 12.8

Image not found

Isoprocarb
Measured: 8.91
Predicted: 13.6

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Menthol
Measured: 10.8
Predicted: 23.5

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(1R,2S,5R)-(-)-Menthol
Measured: 10.8
Predicted: 23.5